Torsion 338 [a:1]([NH1,NH2])[a:2]!@;-[CX3:3](=[O:4])([NX3H0,CX4H0,c]) 0.016 **Binned Counts** Gaussian Fit 0.014 **ETKDG Fit** 0.012 -0.010 -Probability per 0.008 -0.006 0.004 0.002 0.000 60 120 180 Torsion (°)